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A note on Smoluchowski's equations with diffusion

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Abstract

We consider an infinite system of reaction–diffusion equations that models aggregation of particles. Under suitable assumptions on the diffusion coefficients and aggregation rates, we show that this system can be reduced to a scalar equation, for which an explicit self-similar solution is obtained. In addition, pointwise bounds for the solutions of associated initial and initial-boundary value problems are provided.

Keywords: Particle aggregation; Reaction–diffusion; Explicit solutions; Supersolution; Subsolution

1. Introduction and model equations

This note concerns the following infinite system of reaction–diffusion equations:

$$\frac{\partial c_j}{\partial t} = D_j \triangle c_j + \frac{1}{2}\sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - \sum_{k=1}^{\infty} a_{j,k} c_j c_k \qquad (j \geq 1), \tag{1}$$

where the second term on the right above is assumed to cancel when $j = 1$. Here $c_j(\mathbf{x}, t)$ denotes the concentration of clusters of j individual particles at a point $\mathbf{x} \in \mathbb{R}^N$ $(N \geq 1)$ and at time $t > 0$ for all $j \geq 1$. The diffusion coefficients D_j $(j \geq 1)$ and aggregation rates $a_{j,k}$ $(j, k \geq 1)$ are such that $D_j \geq 0$ and $a_{j,k} = a_{k,j} \geq 0$ for all $j, k \geq 1$.

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The kinetic version of (1) given by

$$\frac{\mathrm{d}\widehat{c}_j}{\mathrm{d}t} = \frac{1}{2}\sum_{k=1}^{j-1} a_{j-k,k}\widehat{c}_{j-k}\widehat{c}_k - \sum_{k=1}^{\infty} a_{j,k}\widehat{c}_j\widehat{c}_k \qquad (j \geq 1) \tag{2}$$

was derived by Smoluchowski (for a particular choice of $a_{j,k}$ $(j, k \geq 1)$) as a model to describe the coagulation of colloidal particles in a solution [1,2]. Different aggregation rates were later considered to address a number of physical situations [3–6]. For example, in the Flory–Stockmayer theory of polymer formation, the coefficients $a_{j,k}$ $(j, k \geq 1)$ are supposed to depend on the number of functional groups capable of reacting with each other and that are present in each monomeric unit. More specifically, the aggregation rates are taken to be

$$a_{j,k} = (Aj + B)(Ak + B) \qquad (A \geq 0, B \geq 0) \tag{3}$$

for all $j, k \geq 1$. Other choices of such coefficients are discussed in [7].

A remarkable fact concerning (2) is that a number of explicit solutions are known. Two particularly relevant ones are due to Leyvraz and Tschudi [8] (see also [9]) and Leyvraz [7]. The first of these, corresponding to the choices $A = 1$ and $B = 0$ in (3), reads as follows:

$$\begin{aligned} \widehat{c}_j(t) &= \frac{j^{j-3}t^{j-1}\mathrm{e}^{-jt}}{(j-1)!} \qquad \text{for } 0 \leq t \leq 1, \\ &= \frac{j^{j-3}\mathrm{e}^{-j}}{(j-1)!t} \qquad \text{for } 1 < t \end{aligned}$$

for all $j \geq 1$. The (normalized) mass density $\rho(t) = \sum_{j=1}^{\infty} j\widehat{c}_j(t)$ associated with (4) is then such that $\rho(t) = 1$ for $0 \leq t \leq 1$ and $\rho(t) = 1/t$ for $t > 1$. Thus, the mass ceases to be conserved after the so-called gelation time $t_g = 1$. This illustrates the onset of a sol–gel phase transition (see [3,8] and the references therein). A second class of explicit solutions of interest here was obtained in [7] for product aggregation rates $a_{j,k} = r_j r_k$ where $r_j > 0$ for all $j \geq 1$. It was derived from the ansatz

$$\widehat{c}_j(t) = \frac{\alpha_j}{t} \qquad (\alpha_j > 0, j \geq 1). \tag{4}$$

Substituting (4) into (2) yields

$$-\alpha_j = \frac{1}{2}\sum_{k=1}^{j-1} r_{j-k}r_k\alpha_{j-k}\alpha_k - r_j\alpha_j\sum_{k=1}^{\infty} r_k\alpha_k \qquad (j \geq 1). \tag{5}$$

It was shown in [7] that under the assumptions

$$r_j > r_1 > 0 \text{ for all } j \geq 2 \text{ and } \lim_{j\to\infty}\frac{1}{r_j} = 0, \tag{6}$$

the infinite algebraic system (5) has a positive solution α_j $(j \geq 1)$ (see also [10–12]). Hence, (2) possesses a solution of the form (4). When $r_j \geq Bj^{\alpha}$ $(B > 0, \alpha > 1/2)$, such a function does not preserve the mass, so it was referred to as a post-gel solution in [7].

On the other hand, a careful reassessment of Smoluchowski's original assumptions has led to the consideration of the more general reaction–diffusion system (1). For instance, cluster diffusion (as represented by the Laplacian operators in (1)) was introduced in [13] to account for the stochastic exchange of particles between clusters. In [14] a system of the form (1) was obtained as the macroscopic